

=> fil casrea; d stat que l35

FILE 'CASREACT' ENTERED AT 09:44:21 ON 01 JUN 2007

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FILE CONTENT:1840 - 27 May 2007 VOL 146 ISS 23

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*
*      CASREACT now has more than 12 million reactions
*
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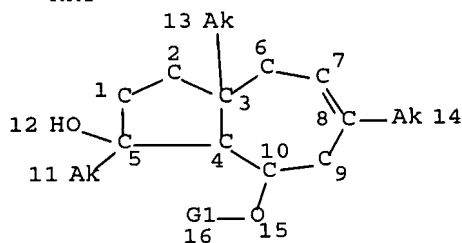
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

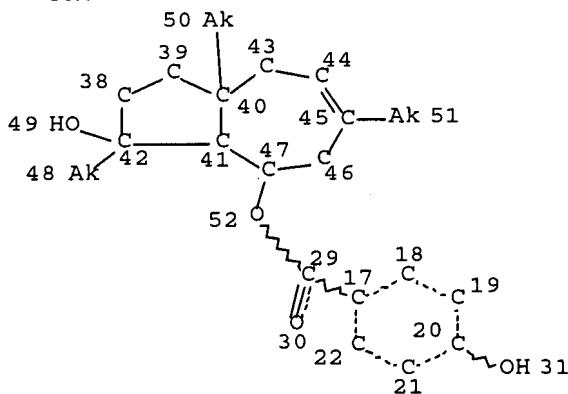
L32

STR

RRT



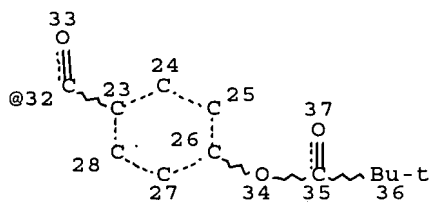
PRO



RRT=REACTANT OR REAGENT

PRO=PRODUCT

Page 1-A



Page 2-A

VAR G1=H/32

NODE ATTRIBUTES:

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CONNECT IS E1 RC AT 13

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 48

CONNECT IS E1 RC AT 50

CONNECT IS E1 RC AT 51

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 11 13 14 48 50 51

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 52

STEREO ATTRIBUTES: NONE

L35 0 SEA FILE=CASREACT SSS FUL L32 (0 REACTIONS)

100.0% DONE 16648 VERIFIED 0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

=> fil reg; d stat que 121; d que nos 122
 FILE 'REGISTRY' ENTERED AT 09:44:44 ON 01 JUN 2007
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Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 31 MAY 2007 HIGHEST RN 936320-32-0
 DICTIONARY FILE UPDATES: 31 MAY 2007 HIGHEST RN 936320-32-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

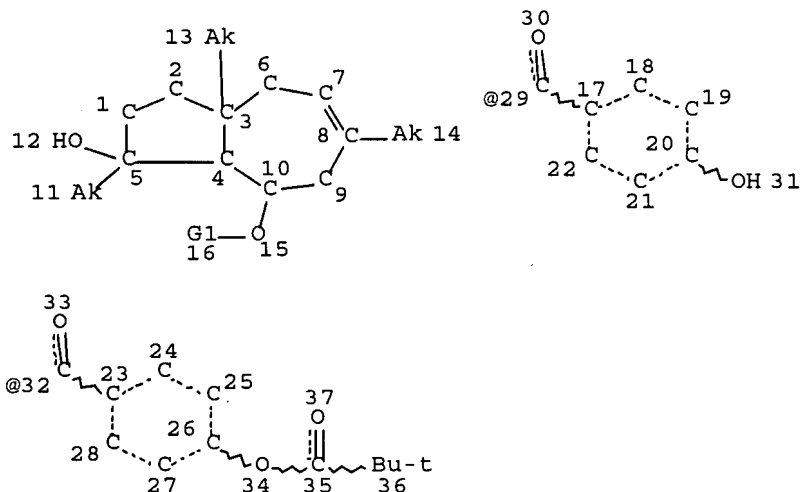
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

L11 STR



VAR G1=H/32/29
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 DEFAULT ECLEVEL IS LIMITED

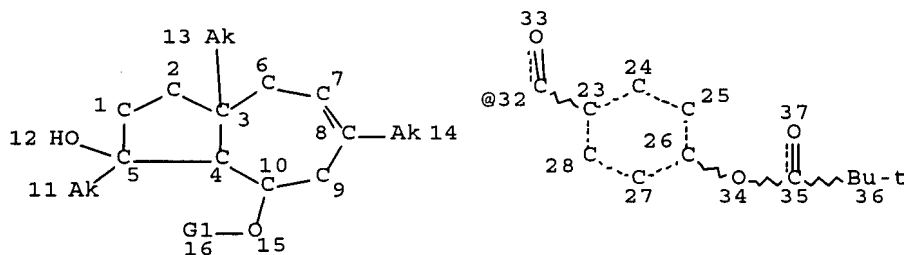
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

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L17 STR



VAR G1=H/32

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MLEVEL IS CLASS AT 11 13 14

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

L21 23 SEA FILE=REGISTRY SUB=L14 SSS FUL L17

100.0% PROCESSED 50 ITERATIONS

23 ANSWERS

SEARCH TIME: 00.00.01

L11 STR

L14 50 SEA FILE=REGISTRY SSS FUL L11

L17 STR

L21 23 SEA FILE=REGISTRY SUB=L14 SSS FUL L17

L22 27 SEA FILE=REGISTRY ABB=ON L14 NOT L21

INVENTOR SEARCH

=> fil capl

FILE 'CAPLUS' ENTERED AT 09:44:54 ON 01 JUN 2007

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FILE COVERS 1907 - 1 Jun 2007 VOL 146 ISS 24

FILE LAST UPDATED: 31 May 2007 (20070531/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> => d que nos l38

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L2          330 SEA FILE=CAPLUS ABB=ON  BOMBARDELLI E?/AU
L3          219 SEA FILE=CAPLUS ABB=ON  FONTANA G?/AU
L4          33 SEA FILE=CAPLUS ABB=ON  CRISTONI A?/AU
L5          9 SEA FILE=CAPLUS ABB=ON  MERCALLI E?/AU
L8          2492 SEA FILE=CAPLUS ABB=ON  FERULA?/OBI
L10         4 SEA FILE=CAPLUS ABB=ON  (L2 OR L3 OR L4 OR L5) AND L8
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L38 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:523306 CAPLUS Full-text

DOCUMENT NUMBER: 143:48133

TITLE: Compositions for the treatment of atopic dermatitis, skin allergic conditions, and acne

INVENTOR(S): Bombardelli, Ezio

PATENT ASSIGNEE(S): Indena S.p.A., Italy

SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005053720	A1	20050616	WO 2004-EP12608	20041108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004294691	A1	20050616	AU 2004-294691	20041108
CA 2546959	A1	20050616	CA 2004-2546959	20041108
EP 1713490	A1	20061025	EP 2004-797704	20041108
EP 1713490	B1	20070418		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1886146	A	20061227	CN 2004-80034658	20041108
BR 2004016846	A	20070213	BR 2004-16846	20041108
AT 359803	T	20070515	AT 2004-797704	20041108
JP 2007512271	T	20070517	JP 2006-540237	20041108
NO 2006002354	A	20060523	NO 2006-2354	20060523
US 2007071839	A1	20070329	US 2006-579966	20060523
PRIORITY APPLN. INFO.:			IT 2003-MI2286	A 20031124
			IT 2003-MI228	A 20031124
			WO 2004-EP12608	W 20041108

ED Entered STN: 17 Jun 2005

AB The present invention relates to topical compns. containing: a) Ginkgo biloba terpenes; b) floroglucinols pure or in mixture thereof, extracted from Humulus lupulus, Hypericum sp. and Myrtus sp.; c) Zanthoxylum bungeanum or Echinacea angustifolia lipophilic extract; for the treatment of atopic dermatitis, skin allergic conditions and acne.

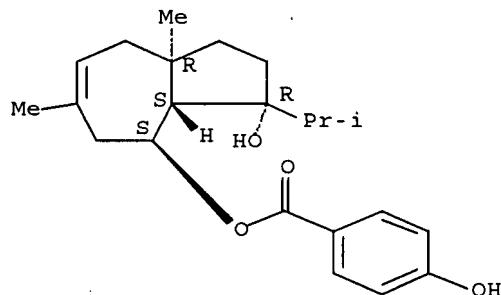
IT 41743-44-6, Ferutinin

RL: NPO (Natural product occurrence); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(herbal compns. for the treatment of atopic dermatitis, skin allergic conditions, and acne)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1024100 CAPLUS Full-text

DOCUMENT NUMBER: 142:130764

TITLE: Antimycobacterial Coumarins from the Sardinian Giant
Fennel (*Ferula communis*)AUTHOR(S): Appendino, Giovanni; Mercalli, Enrico;
Fuzzati, Nicola; Arnoldi, Lolita; Stavri, Michael;
Gibbons, Simon; Ballero, Mauro; Maxia, AndreaCORPORATE SOURCE: Dipartimento di Scienze Chimiche, Alimentari
Farmaceutiche e Farmacologiche, Universita del
Piemonte Orientale, Novara, 28100, ItalySOURCE: Journal of Natural Products (2004), 67(12), 2108-2110
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:130764

ED Entered STN: 30 Nov 2004

AB The structure of a new prenylated coumarin (E- ω -benzoyloxyferulenol, 1b) from the Sardinian giant fennel (*Ferula communis*) has been confirmed by synthesis. The parent compound ferulenol (1a) showed sub-micromolar antimycobacterial activity, which was partly retained in 1b and in the simplified synthetic analog 3, but diminished in its ω -hydroxy and ω -acetoxy derivs. (1c and 1d, resp.). The outstanding activity of 1a, its low toxicity, and the evidence for definite structure-activity relationships make this prenylated 4-hydroxycoumarin an interesting antibacterial chemotype worth further investigation.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:857419 CAPLUS Full-text

DOCUMENT NUMBER: 141:337637

TITLE: A process for the preparation of ferutinin from
Ferula genus plantsINVENTOR(S): Bombardelli, Ezio; Fontana, Gabriele
; Cristoni, Aldo; Mercalli, Enrico

PATENT ASSIGNEE(S): Indena S.P.A., Italy

SOURCE: PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087179	A1	20041014	WO 2004-EP3055	20040323
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,			

TD, TG

AU 2004226853	A1	20041014	AU 2004-226853	20040323
CA 2521100	A1	20041014	CA 2004-2521100	20040323
EP 1615651	A1	20060118	EP 2004-722572	20040323
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004009166	A	20060411	BR 2004-9166	20040323
CN 1767841	A	20060503	CN 2004-80009111	20040323
JP 2006522043	T	20060928	JP 2006-504815	20040323
NO 2005004545	A	20051006	NO 2005-4545	20051003
US 2006275246	A1	20061207	US 2005-551772	20051003 <--
PRIORITY APPLN. INFO.:			IT 2003-MI661	A 20030404
			WO 2004-EP3055	W 20040323

ED Entered STN: 18 Oct 2004

AB The invention relates to a process for the preparation of ferutinin from *Ferula* spp exts. comprising basic hydrolysis of the exts. and treatment with p-pivaloyloxybenzoic acid. The invention relates also to the use of the exts. and ferutinin in the cosmetic and dermatol. field.

IT 41743-44-6P, Ferutinin

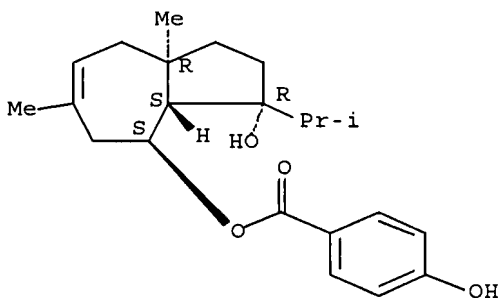
RL: BPN (Biosynthetic preparation); COS (Cosmetic use); NPO (Natural product occurrence); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(process for the preparation of ferutinin from *Ferula* genus plants)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (CA INDEX NAME)

Absolute stereochemistry.



IT 41690-67-9P, Jaeschkenadiol 773115-81-4P

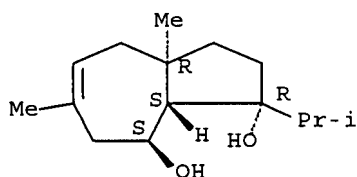
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(process for the preparation of ferutinin from *Ferula* genus plants)

RN 41690-67-9 CAPLUS

CN 1,8-Azulenediol, 1,2,3,3a,4,7,8,8a-octahydro-3a,6-dimethyl-1-(1-methylethyl)-, (1R,3aR,8S,8aS)- (9CI) (CA INDEX NAME)

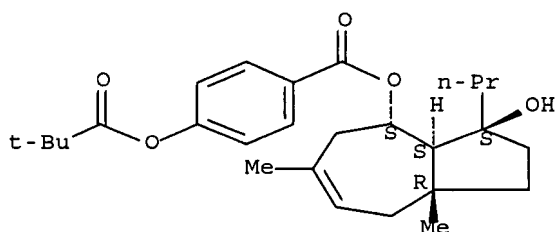
Absolute stereochemistry.



RN 773115-81-4 CAPLUS

CN Benzoic acid, 4-(2,2-dimethyl-1-oxopropoxy)-, (3S,3aS,4S,8aR)-
1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-propyl-4-azulenyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:419939 CAPLUS Full-text

DOCUMENT NUMBER: 142:51707

TITLE: HPLC-DAD-MS identification of bioactive secondary
metabolites from *Ferula communis* roots

AUTHOR(S): Arnoldi, Lolita; Ballero, Mauro; Fuzzati, Nicola;
Maxia, Andrea; Marcalli, Enrico; Pagni, Luca

CORPORATE SOURCE: Indena S.p.A. Research and Development Laboratories,
Settala (MI), 20090, Italy

SOURCE: Fitoterapia (2004), 75(3-4), 342-354

CODEN: FTRPAE; ISSN: 0367-326X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 25 May 2004

AB A simple HPLC method was developed to distinguish between poisonous' and non-
poisonous' chemotypes of *Ferula communis*. The method was performed on a Cp
reverse phase anal. column using a binary eluent (aqueous TFA 0.01%-TFA 0.01%
in acetonitrile) under gradient condition. The two chemotypes showed
different fingerprints. The identification of five coumarins and eleven
daucane derivs. by HPLC-diode array detection (HPLC-DAD) and HPLC-MS is
described. A coumarin, not yet described, was detected.

IT 41690-67-9, Jaesckeandiol 41743-44-6, Ferutinin
54526-95-3, Teferin

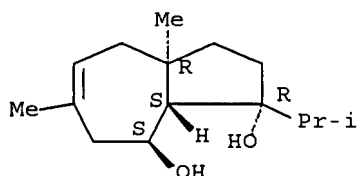
RL: ANT (Analyte); BSU (Biological study, unclassified); NPO (Natural
product occurrence); ANST (Analytical study); BIOL (Biological study);
OCCU (Occurrence)

(identification of bioactive secondary metabolites from *Ferula*
communis roots by HPLC-DAD-MS)

RN 41690-67-9 CAPLUS

CN 1,8-Azulenediol, 1,2,3,3a,4,7,8,8a-octahydro-3a,6-dimethyl-1-(1-methylethyl)-, (1R,3aR,8S,8aS)- (9CI) (CA INDEX NAME)

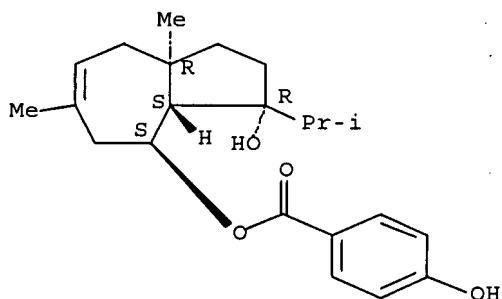
Absolute stereochemistry.



RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (CA INDEX NAME)

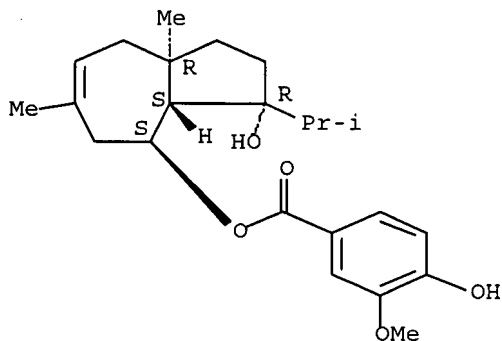
Absolute stereochemistry.



RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

REACTION SEARCH REFERENCES

=> d que nos 126

L11 STR
 L14 50 SEA FILE=REGISTRY SSS FUL L11
 L16 1 SEA FILE=REGISTRY ABB=ON 86068-43-1
 L17 STR
 L21 23 SEA FILE=REGISTRY SUB=L14 SSS FUL L17
 L22 27 SEA FILE=REGISTRY ABB=ON L14 NOT L21
 L23 49 SEA FILE=CAPLUS ABB=ON L21
 L24 14 SEA FILE=CAPLUS ABB=ON L22/P
 L25 6 SEA FILE=CAPLUS ABB=ON L16
 L26 3 SEA FILE=CAPLUS ABB=ON L24 AND (L23 OR L25)

=> s 126 not 138

L39 2 L26 NOT L38

=> d ibib ed abs hitstr 139 1-2; fil hom

L39 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:541439 CAPLUS Full-text

DOCUMENT NUMBER: 141:346209

TITLE: Structure of Samferine

AUTHOR(S): Eshbakova, K. A.; Saidkhodzhaev, A. I.

CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant
Substances, Academy of Sciences of the Republic of
Uzbekistan, Uzbekistan

SOURCE: Chemistry of Natural Compounds (Translation of Khimiya
Prirodnikh Soedinenii) (2004), 40(2), 194-195
CODEN: CHNCA8; ISSN: 0009-3130

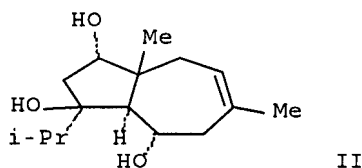
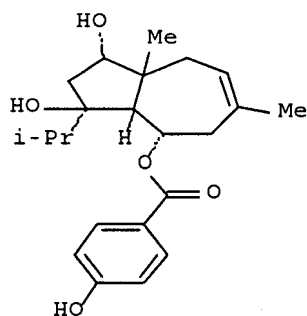
PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 07 Jul 2004

GI



AB The authors have isolated a new compound samferine (I), of formula C₂₂H₃₀O₅, from the roots of *F. samarcandica* Korov. Alkaline hydrolysis of I produced a sesquiterpene alc. samferol (II), of the formula C₁₅H₂₆O₃, from the neutral part of the hydrolyzate.

IT 774577-57-0P, Samferine

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence);

PREP (Preparation); RACT (Reactant or reagent)

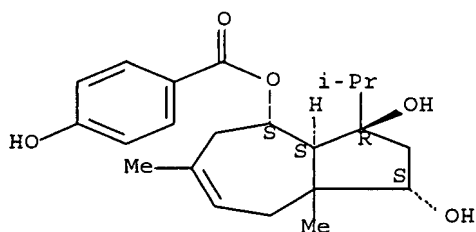
(isolation and mol. structure of sesquiterpene ester samferine from *F. samarcandica*)

RN 774577-57-0 CAPLUS

CN Benzoic acid, 4-hydroxy-, (1R,3S,3aR,4R)-1,2,3,3a,4,5,8,8a-octahydro-1,3-dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.



IT 774577-58-1P, Samferol

RL: SPN (Synthetic preparation); PREP (Preparation)

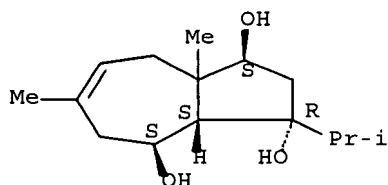
(isolation and mol. structure of sesquiterpene ester samferine from *F. samarcandica*)

RN 774577-58-1 CAPLUS

CN 1,3,4-Azulenetriol, 1,2,3,3a,4,5,8,8a-octahydro-6,8a-dimethyl-3-(1-methylethyl)-, (1R,3S,3aR,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:709827 CAPLUS Full-text

DOCUMENT NUMBER: 137:363261

TITLE: Daucane phytoestrogens: a structure-activity study

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CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Alimentari, Farmaceutiche e Farmacologiche, Universita del Piemonte Orientale, Novara, 28100, Italy

SOURCE: Journal of Natural Products (2002), 65(11), 1612-1615
CODEN: JNPRDF; ISSN: 0163-3864

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LANGUAGE: English

ED Entered STN: 19 Sep 2002

AB The estrogenic activity of a series of analogs of the daucane ester ferutinin modified at the acyl moiety was investigated in a yeast screen containing the human estrogen receptor α . Rather strict structure-activity relationships were observed. Thus, while the parent polyol (jaeschkeanadiol) was inactive, the presence of a p-hydroxybenzoyl moiety was necessary for activity in the yeast screen. Homologation and vinylation were both detrimental for activity, as were methylation of the p-hydroxyl substituent and the introduction of oxygen functions on the adjacent carbons.

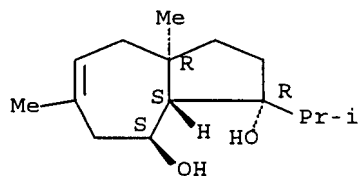
IT 41690-67-9P, Jaeschkeanadiol

RL: PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(daucane phytoestrogens: a structure-activity study)

RN 41690-67-9 CAPLUS

CN 1,8-Azulenediol, 1,2,3,3a,4,7,8,8a-octahydro-3a,6-dimethyl-1-(1-methylethyl)-, (1R,3aR,8S,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 41743-44-6DP, Ferutinin, derivs. 41743-44-6P, Ferutinin

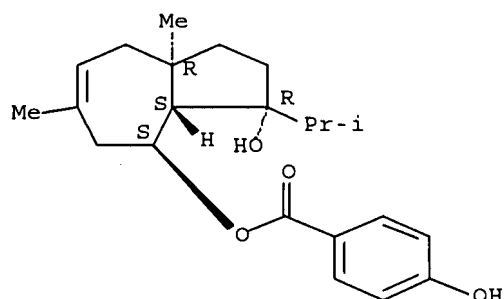
54526-95-3P 126783-56-0P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(daucane phytoestrogens: a structure-activity study)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (CA INDEX NAME)

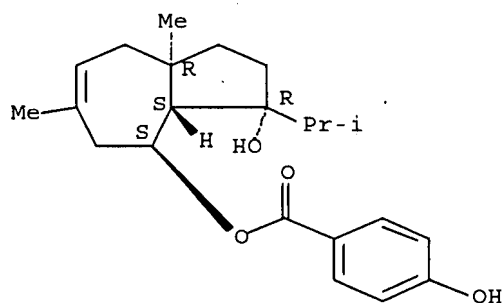
Absolute stereochemistry.



RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (CA INDEX NAME)

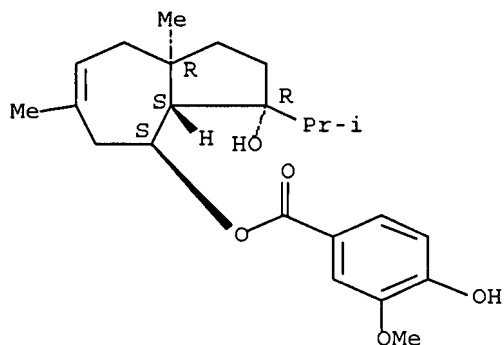
Absolute stereochemistry.



RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI)
(CA INDEX NAME)

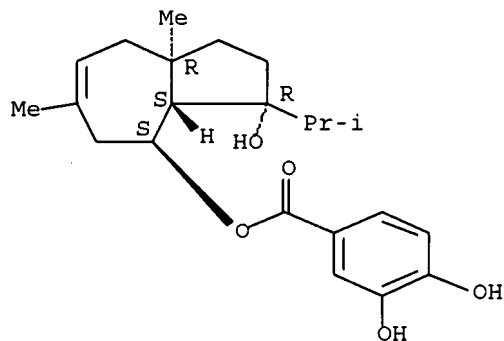
Absolute stereochemistry.



RN 126783-56-0 CAPLUS

CN Benzoic acid, 3,4-dihydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

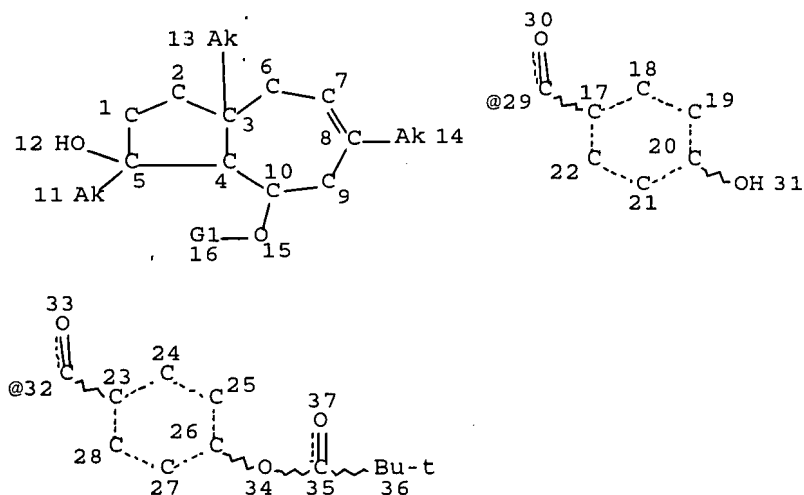
35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

FILE 'HOME' ENTERED AT 09:46:12 ON 01 JUN 2007

SEARCH HISTORY

=> d stat que l21; d his nofile
L11 STR



VAR G1=H/32/29

NODE ATTRIBUTES:

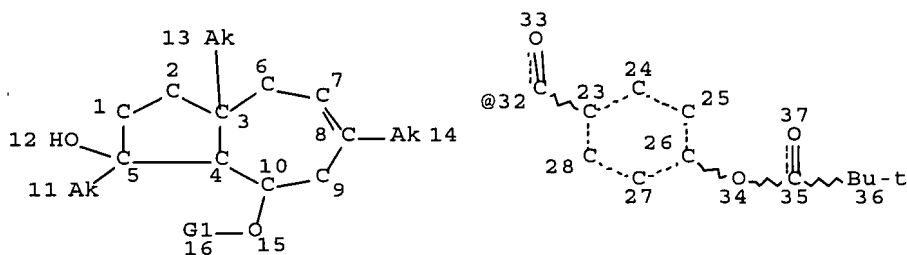
CONNECT IS E1 RC AT 11
CONNECT IS E1 RC AT 13
CONNECT IS E1 RC AT 14
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 11 13 14
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L14 50 SEA FILE=REGISTRY SSS FUL L11
L17 STR



VAR G1=H/32

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 11
CONNECT IS E1 RC AT 13
CONNECT IS E1 RC AT 14
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 11 13 14

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

L21 23 SEA FILE=REGISTRY SUB=L14 SSS FUL L17

100.0% PROCESSED 50 ITERATIONS

23 ANSWERS

SEARCH TIME: 00.00.01

(FILE 'HOME' ENTERED AT 09:25:32 ON 01 JUN 2007)

FILE 'CAPLUS' ENTERED AT 09:26:29 ON 01 JUN 2007

E US2005-551772/APPS

L1 1 SEA ABB=ON US2005-551772/AP
D SCAN
L2 330 SEA ABB=ON BOMBARDELLI E?/AU
L3 219 SEA ABB=ON FONTANA G?/AU
L4 33 SEA ABB=ON CRISTONI A?/AU
L5 9 SEA ABB=ON MERCALLI E?/AU
L6 1 SEA ABB=ON L2 AND L3 AND L4 AND L5
L7 51 SEA ABB=ON (L2 AND (L3 OR L4 OR L5)) OR (L3 AND (L4 OR L5))
OR (L4 AND L5)
L8 2492 SEA ABB=ON FERULA?/OBI
L9 1 SEA ABB=ON L7 AND L8
L10 4 SEA ABB=ON (L2 OR L3 OR L4 OR L5) AND L8

FILE 'REGISTRY' ENTERED AT 09:28:54 ON 01 JUN 2007

L11 STR
L12 2 SEA SSS SAM L11
L13 82752 SEA SSS FUL L11 EXTEND
L14 50 SEA SSS FUL L11
SAVE TEMP L14 KAT772FULL/A

FILE 'CAPLUS' ENTERED AT 09:34:35 ON 01 JUN 2007

L15 98 SEA ABB=ON L14

FILE 'REGISTRY' ENTERED AT 09:34:43 ON 01 JUN 2007

L16 1 SEA ABB=ON 86068-43-1
L17 STR L11
L18 STR L11
L19 0 SEA SUB=L14 SSS SAM L17
D QUE
L20 50 SEA SUB=L14 SSS FUL L17 EXTEND
L21 23 SEA SUB=L14 SSS FUL L17
SAVE TEMP L21 KAT772RRRT/A
L22 27 SEA ABB=ON L14 NOT L21
SAVE TEMP L22 KAT772PRO/A

FILE 'CAPLUS' ENTERED AT 09:38:46 ON 01 JUN 2007

L23 49 SEA ABB=ON L21
L24 14 SEA ABB=ON L22/P
L25 6 SEA ABB=ON L16
L26 3 SEA ABB=ON L24 AND (L23 OR L25)

FILE 'CASREACT' ENTERED AT 09:39:31 ON 01 JUN 2007

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L27      45 SEA ABB=ON  BOMBARDELLI E?/AU
L28      42 SEA ABB=ON  FONTANA G?/AU
L29      1 SEA ABB=ON  CRISTONI A?/AU
L30      1 SEA ABB=ON  MERCALLI E?/AU
L31      18 SEA ABB=ON  ((L29 OR L30) AND (L27 OR L28)) OR (L27 AND L28)
L32      STR L11
L33      0 SEA SSS SAM L32 (      0 REACTIONS)
L34      729 SEA SSS FUL L32 ( 16648 REACTIONS) EXTEND
L35      0 SEA SSS FUL L32 (      0 REACTIONS)
          SAVE TEMP L35 KAT772CASRE/A
          D SCAN L29
          D SCAN L30
L36      0 SEA ABB=ON  (L27 OR L28) AND (L29 OR L30)

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FILE 'CASREACT' ENTERED AT 09:44:21 ON 01 JUN 2007

D STAT QUE L35

FILE 'REGISTRY' ENTERED AT 09:44:44 ON 01 JUN 2007

D STAT QUE L21

D QUE NOS L22

FILE 'CAPLUS' ENTERED AT 09:44:54 ON 01 JUN 2007

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L37      3 SEA ABB=ON  (L2 OR L3 OR L4 OR L5) AND L15
L38      4 SEA ABB=ON  (L37 OR L1 OR L10)
          D QUE NOS L38
          D IBIB ED ABS HITSTR L38 1-4
          D QUE NOS L26
L39      2 SEA ABB=ON  L26 NOT L38
          D IBIB ED ABS HITSTR L39 1-2

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FILE 'HOME' ENTERED AT 09:46:12 ON 01 JUN 2007

D STAT QUE L21

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